Space & time errors estimates in the combined Finite Volume–Exponential integrator for nonlinear reactive transport.

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Abstract

We analyze the finite volume spatial convergence combined with Exponential Time Differencing of order one (ETD1) for temporal discretization of a non linear Advection–Diffusion–reaction equation (ADR) modeling transport in porous media. We derive the L^2 estimate under the assumption that the non linear reaction is globally Lipschitz. We illustrate the theoretical proof by some applications in 2D and 3D highly anisotropic and heterogeneous porous media including the SPE10 case [1]. We compute the exponential of the non diagonal matrices arriving in the finite volume spatial discretization with the Fast Léja points technique and the Krylov subspace technique.

Keywords: Finite volume, Exponential integrator, Porous media, Advection–diffusion–reaction

1. Introduction

Flow and transport are fundamental in many geo-engineering applications, including oil and gas recovery from hydrocarbon reservoirs, groundwater contamination and sustainable use of groundwater resources, storing greenhouse gases (e.g. CO_2) or radioactive waste in the subsurface, or mining heat from geothermal reservoirs. In porous media, a single phase transport process is described by the equation

$$\phi(\mathbf{x})\frac{\partial X}{\partial t} = \nabla\cdot(\mathbf{D}(\mathbf{x})\nabla X) - \nabla\cdot(\mathbf{q}(\mathbf{x})X) + R(t,\mathbf{x},X) \quad (\mathbf{x},t) \in \Omega\times[0,T]\,, \quad (1)$$

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where Ω is an open domain of $\mathbb{R}^d$, $d \in \{1, 2, 3\}$, ϕ is the porosity (void fraction) of the rock, and $\mathbf{D}$ is the symmetric dispersion tensor, X is the unknown concentration of the contaminant, $\mathbf{q}$ the Darcy's velocity and R the reaction and source term.
Finite element, finite volume or the combination finite element-finite volume methods are mostly used for space discretization of the problem (1) while explicit Euler, semi implicit and fully implicit methods are usually used for time discretization [5, 7, 9, 10]. Due to time step size constraints, fully implicit scheme is more popular for time discretization for quite a long time compared to explicit Euler and semi implicit methods. This method, however, need at each time step a solution of large systems of nonlinear equations. This can be the bottleneck in computations. In recent years, exponential integrators have become an attractive alternative in many evolutions equations [2, 3, 4, 19, 6, 11, 12, 17, 20, 11, 12, 14]. In contrast to classical methods, they do not require the solution of large linear systems. Instead they make explicit use of the matrix exponential and related matrix functions. The price to pay is the computing of the matrix exponential functions of the non diagonal matrices, which has revived interest and significance progresses nowadays [6, 19, 11, 12, 20, 11, 12].

In this work, we combine a finite volume method with the first order exponential time differencing scheme of order 1 (ETD1). Although both discretization techniques have been together used for solving evolutionary problems like (1) (see [2, 3, 4]), a proper combination of rigorous proof of them has been lacking so far.

The paper is organised as follows. In Section 2 we present the semi group formulation. In Section 3 and Section 4 we present the space and time discretization. We then state and discuss our main result in Section 5 and present the proof of the convergence theorem. We end by presenting some simulations in Section 6, these are applied both to a linear example where we can compute an exact solution as well as a more realistic model (SPE10 case [1]).

2. Semi group formulation and well posedness

Let us start by presenting briefly the notation of the main function spaces and norms that we use in this paper. We denote by $\|\cdot\|$ the norm associated to the inner product $(\cdot,\cdot)$ of the Hilbert space $H = L^2(\Omega)$. For a Banach space $\mathcal{V}$ we denote by $\|\cdot\|_{\mathcal{V}}$ the norm of $\mathcal{V}$ and $L(\mathcal{V})$ the set of bounded linear mapping

from $\mathcal{V}$ to $\mathcal{V}$ to $\mathbb{C}$. For the sake of simplicity, without loss of generality we use the homogeneous Dirichlet boundary condition and assume that the porosity ϕ is constant. During our simulation, we will also investigate the general boundary conditions and non constant porosity ϕ. We assume that the Darcy velocity $\mathbf{q}$ is known, and satisfies the following mass conservation for incompressible fluids $\nabla \cdot \mathbf{q} = 0$. The model problem (1) is reformulated as: find the concentration $X(t) \in H^1(\Omega)$ such that

$$\begin{cases} \partial X/\partial t + AX = R(\mathbf{x}, t, X) & (\mathbf{x}, t) \in \Omega \times [0, T] \\ X(\mathbf{x}, 0) = X_0 & \mathbf{x} \in \Omega \\ X(\mathbf{x}, t) = 0 & (\mathbf{x}, t) \in \partial\Omega \times [0, T] \end{cases} \tag{2}$$

where

$$\begin{aligned} AX \equiv A(\mathbf{x}, X) &= -\nabla \cdot (\mathbf{D}\nabla X) + \nabla \cdot (\mathbf{q}(\mathbf{x})X) \\ &= -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_i} \left(D_{i,j}(\mathbf{x})(\frac{\partial X}{\partial x_j} \right) + \sum_{i=1}^{d} q_i(\mathbf{x}) \frac{\partial X}{\partial x_i} + (\nabla \cdot \mathbf{q})\, X \\ &= -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_i} \left(D_{i,j}(\mathbf{x}) \frac{\partial X}{\partial x_j} \right) + \sum_{i=1}^{d} q_i(\mathbf{x}) \frac{\partial X}{\partial x_i}. \end{aligned}$$

For well posedness of (2), we assume that $\mathbf{D}$ is symmetric, $D_{i,j} \in L^\infty(\Omega), q_i \in L^\infty(\Omega)$ and there exists a positive constant $c_1 > 0$ such that

$$\sum_{i,j=1}^{d} D_{i,j}(\mathbf{x})\xi_i\xi_j \geq c_1|\xi|^2 \qquad \forall \xi \in \mathbb{R}^d \quad \mathbf{x} \in \overline{\Omega} \quad c_1 > 0. \tag{3}$$

Set $V = H_0^1(\Omega)$, the bilinear form associated to the operator A is given by

$$a(u, v) = \int_\Omega \left(\sum_{i,j=1}^{d} D_{i,j} \frac{\partial u}{\partial x_j} \frac{\partial v}{\partial x_i} + \sum_{i=1}^{d} q_i \frac{\partial u}{\partial x_j} v \right) dx \qquad u, v \in V. \tag{4}$$

According to Gårding' s inequality (see [19, 21]), there exists two positive constants c_0 and λ_0 such that

$$a(v, v) + c_0\|v\|^2 \geq \lambda_0\|v\|^2_{H^1(\Omega)} \qquad \forall v \in V. \tag{5}$$

By adding $c_0 X$ in both side of the first equation of (1) we have a new operator that we still call A corresponding to the new bilinear form that we still call a such that the following coercivity property holds

$$a(v,v) \geq \lambda_0 \|v\|^2_{H^1(\Omega)} \qquad \forall v \in V. \tag{6}$$

We will still call the right hand side of the first equation of (2) R.

By Green's formula we have

$$a(u,v) = (Au, v) \qquad \forall u \in H_0^1 \cap H^2(\Omega) = \mathcal{D}(A), \qquad \forall v \in V, \tag{7}$$

where $\mathcal{D}(A)$ the domain of the operator A. Therefore the weak form of (2) is to find the function $X(t) \in \mathcal{D}(A)$ such that

$$\begin{cases} (X_t, \chi) + (AX, \chi) = (R(X), \chi) & \forall \chi \in V, \quad t \in [0,T] \\ X(t) = X_0. \end{cases} \tag{8}$$

The $V-$ellipticity (6) implies that $-A$ is a sectorial on $L^2(\Omega)$ (see [23, 21]) i.e. there exists C_1, $\theta \in (\frac{1}{2}\pi, \pi)$ such that

$$\|(\lambda I + A)^{-1}\|_{L(L^2(\Omega))} \leq \frac{C_1}{|\lambda|} \qquad \lambda \in S_\theta, \tag{9}$$

where $S_\theta = \left\{\lambda \in \mathbb{C} : \lambda = \rho e^{i\phi},\ \rho > 0,\ 0 \leq |\phi| \leq \theta\right\}$.

Then $-A$ is the infinitesimal generator of bounded analytic semigroups $S(t) := e^{-tA}$ on $L^2(\Omega)$ such that

$$S(t) := e^{-tA} = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{t\,\lambda} (\lambda I + A)^{-1} d\lambda, \qquad t > 0 \tag{10}$$

where $\mathcal{C}$ denotes a path that surrounds the spectrum of $-A$.

The coercivity property in (6) implies also that the set of the real part of the spectrum of A is non negative, which allows the definition of the fractional power of A as: for any $\alpha > 0$

$$\begin{cases} A^{-\alpha} = \dfrac{1}{\Gamma(\alpha)} \int_0^\infty t^{\alpha-1} e^{-At} dt \\ \\ A^{\alpha} = (A^{-\alpha})^{-1} \end{cases} \tag{11}$$

where $\Gamma(\alpha)$ is the Gamma function of α [23]. We denote by $\|.\|_\alpha := \|A^{\alpha/2}.\|$ the norm of the space $\mathcal{D}(A^{\alpha/2})$.

For the nonlinear reaction term we make the following assumption

Assumption 2.1. ***[Lipschitz condition for*** R***]***
The nonlinear R *is continuous and differentiable respect to* X *with respect to the variable* X*, with bounded differential. Therefore there exists a positive constant* $L > 0$ *such that*

$$\begin{cases} |R(\mathbf{x},t,u) - R(\mathbf{x},t,v)| \leq L|u-v| \quad \forall u,v \in \mathbb{R}, \quad \mathbf{x} \in \overline{\Omega}, \quad t \in [0,T] \\ \\ \|R(Y) - R(Z)\| \leq L\|Y - Z\| \quad \forall Y,Z \in L^2(\Omega), \end{cases} \tag{12}$$

where with a slight abuse of notation, R denotes the nonlinear operator $X \to R(\cdot,\cdot,X)$.

By Duhamel's principle we may represent solutions of (2) by the following integral equation

$$X(t) = S(t)X_0 + \int_0^t S(t-s)R(s,X(s))ds, \qquad t \in [0,T]\,. \tag{13}$$

Applying the contraction mapping principle in the topology of the Banach space $C([0,T],H^1(\Omega))$ to the integral equation (13) [23, Theorem 3.3.3] or [22, Theorem 6.3.1] ensure the existence and uniqueness of X.

3. Finite volume for space discretization

A cell–centred finite volume methods for heterogeneous and anisotropic diffusion problems remains a challenging problem. An active area of research is to make the approximation of the diffusion flux more efficient and simple as possible (see [24] for the references). The finite volume method is widely applied when the differential equations are in divergence form. To obtain a finite volume discretization, the domain Ω is subdivided into subdomains $(A_i)_{i\in\mathcal{I}}$, $\mathcal{I}$ being the corresponding set of indices, called control volumes or control domains such that the collection of all those subdomains forms a partition of Ω. The common feature of all finite volume methods is to integrate the equation over each control volume A_i, $i \in \mathcal{I}$ and apply Gauss's divergence theorem to convert the volume integral to a surface integral. For our parabolic problem (2), finite volume methods differ in the way they approximate the diffusion flux $F = -\mathbf{D}\nabla X$. Two techniques are mostly used: the finite volume with two-point flux approximation (TPFA) (see [7, 24]) and the finite volume with multi-point flux approximations (MPFA)([25, 26]).

An advantage of the two-point approximation is that it provides monotonicity properties, under the form of a local maximum principle. It is efficient and mostly used in industrial simulations. In this paper we use the TPFA as developed in [7, section 11 page 815]. The main drawback of TPFA is that it is applicable in the so called " admissible mesh " and not in general mesh.

Definition 3.1. *[**An admissible mesh [7]**]*

An admissible mesh $\mathcal{T}$ for problem (2) with the full diffusion tensor $\mathbf{D}$ is given by:

- *A set $\{A_i\}_{i\in\mathcal{I}}$ of control volumes such that $\overline{\Omega} = \underset{i\in\mathcal{I}}{\cup}\overline{A_i}$ with the corresponding local inner product induced by $\mathbf{D}_{A_i}^{-1}$ where*

$$\mathbf{D}_{A_i} = \frac{1}{\mathrm{mes}(A_i)}\int_{A_i}\mathbf{D}(\mathbf{x})d\mathbf{x}.$$

- *The corresponding set of center points $\{\mathbf{x}_i\}_{i\in\mathcal{I}}$ such that*
  - *(a) $\mathbf{x}_i \in \overline{A}_i,\ i \in \mathcal{I}$.*
  - *(b) $\mathbf{x}_i$ is the intersection of the straight lines perpendicular to the boundary of A_i with respect to the inner product induced by $\mathbf{D}_{A_i}^{-1}$.*

Let h be the maximum mesh size of $\mathcal{T}$. We denote by $\mathcal{T}_h$ a dual Delaunay triangulation of $\mathcal{T}$ i.e. the Delaunay triangulation where $\{\mathbf{x}_i\}_{i\in\mathcal{I}}$ is the set of vertices.

Let us illustre Definition 3.1 to make it more understandable.

Example 1.

- *In the case where the diffusion tensor $\mathbf{D}$ is diagonal and Ω is a rectangular or parallelepiped domain, any rectangular grid ($d = 2$) or parallelepiped grid ($d = 3$) is an admissible mesh. The set $\{\mathbf{x}_i\}$ is the set of centers of gravity of the rectangular grid or parallelepiped grid. The inner product induced locally by $\mathbf{D}_{A_i}^{-1}$ is equivalent to the standard inner product corresponding to the Euclidean norm $|.|$. This mesh will yield a 5-point scheme ($d = 2$) and 7-point scheme ($d = 3$) for our model problem (2).*

- *If $d = 2$, for isotropic and heterogeneous media ($\mathbf{D}(\mathbf{x}) = b(\mathbf{x})I_2$ $\mathbf{x} \in \Omega$, I_2 being the identity matrix of dimension 2) we can define a triangular*

admissible mesh $\mathcal{T}$ to be a family of open triangular disjoint subsets of Ω such that two triangles having a common edge have also two common vertices. The angles of the triangles are assumed to be less than $\frac{\pi}{2}$ to allow the orthogonal bisectors to intersect inside each triangle, thus naturally defining the center point $\mathbf{x}_i$ of the control volume A_i. The finite volume scheme defined on such mesh will yield a 4-point scheme for our model problem (2). The inner product induced locally by $\mathbf{D}_{A_i}^{-1}$ is equivalence to the standard inner product corresponding to the Euclidean norm $|.|$.

To make notation easier, we will identify $\mathcal{T}$ to $\mathcal{I}$, then to say $A_i \in \mathcal{T}$ we will say $i \in \mathcal{T}$.

Consider the modified model problem of (2) where $c_0 X$ is added on both sides of the first equation of problem (2), c_0 is defined in (5). Consider an admissible mesh $\mathcal{T}$ in the sense of Definition 3.1. Denote by $\mathcal{E}$ the set of edges of control volume of $\mathcal{T}$, $\mathcal{E}_{int}$ the set of interior edges of control volume of $\mathcal{T}$, $X_i(t)$ the approximation of X at time t at the center (or at any point) of the control volume $i \in \mathcal{T}$ and $X_\sigma(t)$ the approximation of X at time t at the center (or at any point)of the edge $\sigma \in \mathcal{E}$. For a control volume $i \in \mathcal{T}$, denote by $\mathcal{E}_i$ the set of edges of i, mes(i) the Lebesgue measure of the control volume $i \in \mathcal{T}$.

As in [7, 27], integration over any control volume $i \in \mathcal{T}$, using the divergence theorem to convert the integral over i to a surface integral, finite differences for the diffusion flux approximation [7] and the upwind technique for the advection flux approximation yields

$$\begin{cases} \operatorname{mes}(i)\dfrac{dX_i(t)}{dt} + \displaystyle\sum_{\sigma\in\mathcal{E}_i} \left(F_{i,\sigma}(t) + q_{i,\sigma}X_{\sigma,+}(t)\right) + c_0 \operatorname{mes}(i)X_i(t) \\ \qquad\qquad\qquad\qquad\qquad\qquad = \operatorname{mes}(i)\, R(\mathbf{x}_i, t, X_i(t)), \\ D_{i,\sigma} = |\mathbf{D}_i\, \mathbf{n}_{i,\sigma}|, \quad \mathbf{D}_i = \dfrac{1}{\operatorname{mes}(i)} \int_i \mathbf{D}(\mathbf{x}) d\mathbf{x}, \\ F_{i,\sigma}(t) = \operatorname{mes}(\sigma)\; D_{i,\sigma} \dfrac{X_\sigma(t) - X_i(t)}{d_{i,\sigma}}, \\ q_{i,\sigma} = \int_\sigma \mathbf{q}\cdot\mathbf{n}_{i,\sigma} d\sigma \qquad\qquad \forall i \in \mathcal{T},\ \ \forall \sigma \in \mathcal{E}_i. \end{cases} \tag{14}$$

Here $\mathbf{n}_{i,\sigma}$ is the normal unit vector to σ outward to i, mes(σ) is the Lebesgue

measure of the edge $\sigma \in \mathcal{E}_i$ and $d_{i,\sigma}$ the distance between the center of i and the edge σ.

Since the flux is continuous at the interface of two control volumes i and j (denoted by $i \mid j$) we therefore have $F_{i,\sigma}(t) = -F_{j,\sigma}(t)$ for $\sigma = i \mid j$, which yields

$$\begin{cases} F_{i,\sigma}(t) = -\tau_\sigma \left(X_j(t) - X_i(t)\right) = -\dfrac{\mu_\sigma \,\mathrm{mes}(\sigma)}{d_{i,j}} \left(X_j(t) - X_i(t)\right), \; \sigma = i \mid j \\ \tau_\sigma = \mathrm{mes}(\sigma) \dfrac{D_{i,\sigma} D_{j,\sigma}}{D_{i,\sigma}\; d_{i,\sigma} + D_{j,\sigma} d_{j,\sigma}} \quad \text{(transmissibility through } \sigma) \end{cases} \tag{15}$$

with

$$\mu_\sigma = d_{i,j} \frac{D_{i,\sigma} D_{j,\sigma}}{D_{i,\sigma}\; d_{i,\sigma} + D_{j,\sigma} d_{j,\sigma}}, \tag{16}$$

where $d_{i,j}$ is the distance between the center of i and center of j. We will also denote by d_σ the distance $d_{i,j}$ or $d_{i,\sigma}$ for $\sigma = i \mid j$ or $\sigma = \mathcal{E}_i \cap \partial\Omega$ respectively.

Notice that for $\sigma \subset \partial\Omega$, we can also write

$$\begin{aligned} F_{i,\sigma}(t) &= -\tau_\sigma \left(X_j(t) - X_i(t)\right) \\ &= -\frac{\mathrm{mes}(\sigma)\mu_\sigma}{d_{i,\sigma}} \left(X_j(t) - X_i(t)\right) \end{aligned}$$

with

$$\begin{cases} X_j(t) = X_\sigma(t) = 0 \\ \tau_\sigma = \dfrac{\mathrm{mes}(\sigma) D_{i,\sigma}}{d_{i,\sigma}} \\ \mu_\sigma = D_{i,\sigma} \end{cases} \tag{17}$$

The upwind term for advection flux $X_{\sigma,+}$ is defined as

$$X_{\sigma,+}(t) = \begin{cases} X_i(t) & \text{if} \quad q_{i,\sigma} \geqslant 0 \\ X_j(t) & \text{if} \quad q_{i,\sigma} < 0 \end{cases} \quad \text{for} \quad \sigma = i \mid j \tag{18}$$

$$X_{\sigma,+}(t) = \begin{cases} X_i(t) & \text{if} \quad q_{i,\sigma} \geqslant 0 \\ X_\sigma(t) & \text{if} \quad q_{i,\sigma} < 0 \end{cases} \quad \text{for} \;\; \sigma \in \mathcal{E}_i \cap \partial\Omega. \tag{19}$$

We can write $X_{\sigma,+}$ as

$$X_{\sigma,+} = r_\sigma X_i(t) + (1 - r_\sigma) X_j(t), \quad \sigma = i \mid j \tag{20}$$

where $r_\sigma = \dfrac{1}{2}(\text{sign}(q_{i,\sigma}) + 1)$.

The finite volume space discretization for the model problem (2) is given by

$$\begin{cases} \text{mes}(i)\dfrac{dX_i(t)}{dt} + \sum\limits_{\sigma\in\mathcal{E}_i} \Bigg(-\dfrac{\text{mes}(\sigma)\,\mu_\sigma}{d_{i,j}}\,(X_j(t) - X_i(t)) \\ \\ +q_{i,\sigma}\,(r_\sigma X_i(t) + (1-r_\sigma)X_j(t))\Bigg) + c_0\,\text{mes}(i)X_i(t) = \text{mes}(i)R(\mathbf{x}_i, t, X_i(t)) \\ \\ X_j(t) = 0,\ d_{i,j} = d_{i,\sigma} \qquad\qquad \text{if } \sigma\subset\partial\Omega, \quad \forall i\ \in\mathcal{T}. \end{cases} \tag{21}$$

The scheme (21) clearly indicates the affinity of the finite volume method to the finite difference method. However, for the subsequent analysis it is more convenient to rewrite scheme (21) in a discrete variational form.

Multiplying the first equation of (21) by arbitrary numbers $v_i \in \mathbb{R}$ and summing the results over all control volume in $\mathcal{T}$ yields

$$\begin{cases} \sum\limits_{i\in\mathcal{T}} \Bigg[\text{mes}(i)\dfrac{dX_i(t)}{dt} + \sum\limits_{\sigma\in\mathcal{E}_i} \Bigg(\dfrac{\text{mes}(\sigma)\,\mu_\sigma}{d_{i,j}}\,(X_i(t) - X_j(t)) \\ \\ +q_{i,\sigma}\,(r_\sigma X_i(t) + (1-r_\sigma)X_j(t))\Bigg)\Bigg]\,v_i = \sum\limits_{i\in\mathcal{T}}\text{mes}(i)\,R(X_i(t))v_i, \\ \\ R(X_i(t)) := R(\mathbf{x}_i, t, X_i(t)). \end{cases} \tag{22}$$

Let $V_h \subset V$ denote the space of continuous functions that are piecewise linear over the Delaunay triangulation $\mathcal{T}_h$ (dual of $\mathcal{T}$), then the values $X_i(t)$ and v_i can be interpolated in V_h. There are unique functions $X_h(t), v_h \in V_h$ such that $X_h(t)(\mathbf{x}_i) = X_i(t)$ and $v_h(\mathbf{x}_i) = v_i$ for all $i \in \mathcal{T}$, where $\mathbf{x}_i$ is a center of the control volume $i \in \mathcal{T}$ ($\mathbf{x}_i$ is also a vertex in $\mathcal{T}_h$).

Denote by a_h the bilinear form defined by

$$\begin{cases} a_h(u_h, v_h) = \sum\limits_{i\in\mathcal{T}}\sum\limits_{\sigma\in\mathcal{E}_i} \Bigg(-\dfrac{\text{mes}(\sigma)\,\mu_\sigma}{d_{i,j}}\,(u_j - u_i) + q_{i,\sigma}\,(r_\sigma u_i + (1-r_\sigma)u_j)\Bigg)\,v_i \\ \\ \qquad +c_0\,\text{mes}(i)u_iv_i \qquad\qquad \forall u_h, v_h \in V_h, \end{cases} \tag{23}$$

and by $\langle .,. \rangle_{0,h}$ the scalar product on $C(\overline{\Omega}) \supset V_h$ defined by

$$\langle u, v \rangle_{0,h} = \sum_{i \in \mathcal{T}} \text{mes}(i) u_i v_i, \quad u_i = u(\mathbf{x}_i), \quad v_i = v(\mathbf{x}_i), \qquad u, v \in C(\overline{\Omega}). \quad (24)$$

The corresponding norm is the discrete $L^2(\Omega)$ norm denoted by $\|.\|_{0,h}$. It is proved in [27] that $\|.\|_{0,h}$ is equivalent to the $L^2(\Omega)$ norm $\|.\|$ in V_h when the mesh $\mathcal{T}$ is regular.
Previous results allow us to write the following variational form of our finite volume scheme (22).

$$\begin{cases} \langle \frac{d}{dt} X_h, \varphi \rangle_{0,h} + a_h(X_h(t), \varphi) = \langle R(X_h(t)), \varphi \rangle_{0,h}, \quad \forall \varphi \in V_h, \quad t \in (0, T], \\ X_h(0) = X_{h\,0}, \end{cases} \quad (25)$$

with

$$R(X_h)(t)(\mathbf{x}_i) = R(X_i(t)) := R(\mathbf{x}_i, t, X_i(t)) = R(\mathbf{x}_i, t, X_h(t)(\mathbf{x}_i)), \qquad \forall i \in \mathcal{T}.$$

Consider the operator $A_h : V_h \to V_h$ such that

$$\langle A_h \psi, \chi \rangle_{0,h} = a_h(\psi, \chi) \quad \forall \psi, \chi \in V_h. \quad (26)$$

The semidiscrete solution in V_h is then given by: find $X_h(t) \in V_h$ such that

$$\begin{cases} \frac{dX_h}{dt} + A_h X_h = P_h R(X_h) \qquad t \in (0, T] \\ X_h(0) = X_{0h} \end{cases} \quad (27)$$

where P_h is the orthogonal projection defined from $u \in C(\overline{\Omega})$ to V_h by

$$\langle P_h u, \chi \rangle_{0,h} = \langle u, \chi \rangle_{0,h} \quad \forall \chi \in V_h. \quad (28)$$

4. Exponential integrator for time discretization

In order to give the corresponding mild form of (27) and build the exponential integrator scheme let us define the discrete $H_0^1(\Omega)$ norm.

Definition 4.1. ***[Discrete*** $H_0^1(\Omega)$ ***norm [7]]***
Let $\mathcal{T}$ be an admissible finite volume mesh in the sense of Definition 3.1. Let $X(\mathcal{T})$ be the space of the functions constant in each control volume of $\mathcal{T}$. For $u \in X(\mathcal{T})$, the discrete $H_0^1(\Omega)$ norm of u is defined by

$$\|u\|_{1,\mathcal{T}} = \left(\sum_{\sigma\in\mathcal{E}} \tau'_\sigma \left(D_\sigma u\right)^2\right)^{1/2} \tag{29}$$

where

$$\begin{aligned} \tau'_\sigma &= \frac{mes(\sigma)}{d_\sigma} \\ D_\sigma u &= |u_i - u_j| \qquad \text{if} \qquad \sigma = i|j \in \mathcal{E}_{int} \\ D_\sigma u &= |u_i| \qquad \text{if} \qquad \sigma \in \partial\Omega. \end{aligned}$$

During our analysis we make the following assumption as in [7, section 11 page 815].

Assumption 4.2. *[**Regularity of** $\mathbf{D}$**,** $\mathbf{q}$ **and the admissible mesh** $\mathcal{T}$]*
We assume that $\mathbf{D}$ is bounded, the restriction of $\mathbf{D}$ to any $i \in \mathcal{T}$ belongs to $C^1(i, \mathbb{R}^{d\times d})$, $q_j \in C^1(\overline{\Omega})$ and that there exists $\zeta_1 > 0$ and $\zeta_2 > 0$ such that

$$\begin{cases} \zeta_1 h^2 \leq \text{mes}(i) \leq \zeta_2 h^2, & \forall i \in \mathcal{T}, \\ \zeta_1 h \leq \text{mes}(\sigma) \leq \zeta_2 h, & \forall \sigma \in \mathcal{E} \\ \zeta_1 h \leq d_\sigma \leq \zeta_2 h, & \forall \sigma \in \mathcal{E}. \end{cases} \tag{30}$$

Assumption 4.2 allows the following V_h- ellipticity of a_h.

Theorem 4.3. *Under the regularity of the admissible mesh $\mathcal{T}$ in Assumption 4.2, there exists a constant $\alpha > 0$ such that*

$$a_h(v_h, v_h) \geq \alpha \left\|v_h\right\|_{1,\mathcal{T}}^2 \quad \forall v_h \in V_h. \tag{31}$$

Proof. Let b_h^1, b_h^2 and b_h^3 the bilinear forms defined in $V_h \times V_h$ by

$$b_h^1(u_h, v_h) = \sum_{i\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_i} - \frac{\text{mes}(\sigma)\,\mu_\sigma}{d_{i,j}} \left(u_j - u_i\right) v_i, \tag{32}$$

$$b_h^2(u_h, v_h) = \sum_{i\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_i} q_{i,\sigma} \left(r_\sigma u_i + (1 - r_\sigma) u_j\right) v_i = \sum_{i\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_i} q_{i,\sigma} u_{\sigma,+} v_i, \tag{33}$$

$$b_h^3(u_h, v_h) = c_0 \sum_{i\in\mathcal{T}} \text{mes}(i)\, u_i v_i. \tag{34}$$

Using Assumption 4.2, mainly the regularity of $\mathcal{T}$ and the fact that the coefficients of the diffusion tensor $\mathbf{D}$ are bounded, there exists two constants $C_5(\Omega, \zeta_1, \zeta_2, \mathbf{D})$ and $C_5'(\Omega, \zeta_1, \zeta_2, \mathbf{D})$ such that

$$C_5 \leq \mu_\sigma = d_{i,j} \frac{D_{i,\sigma} D_{i,\sigma}}{D_{i,\sigma}\ d_{i,\sigma} + D_{i,\sigma} d_{i,\sigma}} \leq C_5', \qquad \sigma = i|j, \tag{35}$$

and

$$C_5 \leq \mu_\sigma = D_{i,\sigma} \leq\ C_5', \qquad \sigma \in \mathcal{E}_i \cap \partial\Omega, \tag{36}$$

so that

$$C_5 \leq \mu_\sigma\ \leq\ C_5'\,, \qquad \forall \sigma \in \mathcal{E}, \tag{37}$$

where μ_σ is defined in (17) and (16).

Using the fact that the transmissibility given in (15) is symmetric, i.e. $\tau_{i|j} = \tau_{j|i}$ and reorganizing the summation, we therefore have

$$C_5 \left\| v_{_h} \right\|_{1,\mathcal{T}}^2 \leq b_h^1(v_h, v_h) \leq C_5' \left\| v_{_h} \right\|_{1,\mathcal{T}}^2 \tag{38}$$

Let use some important results from [7]. Indeed as in [7] reordering the summation over the set of edges yields

$$b_h^2(v_h, v_h) = \sum_{\sigma\in\mathcal{E}} q_\sigma \left(v_{\sigma,+} - v_{\sigma,-}\right) v_{\sigma,+} \tag{39}$$

where

$$\begin{aligned} v_{\sigma,-} \quad &= \quad \begin{cases} v_i \quad \text{if} \quad q_{i,\sigma} \leq 0 \\ \\ v_j \text{ (or } v_\sigma) \quad \text{if} \quad q_{i,\sigma} > 0 \end{cases} \qquad \sigma\ \in \mathcal{E}_{int}\,(\text{or } \sigma \in \mathcal{E}_i \cap \partial\Omega), \qquad (40) \\ q_\sigma \quad &= \quad |\int_\sigma \mathbf{q} \cdot \mathbf{n}_{i,\sigma} d\sigma|. \qquad (41) \end{aligned}$$

Since

$$\sum_{\sigma\in\mathcal{E}} q_\sigma \left(v_{\sigma,+} - v_{\sigma,-}\right) v_{\sigma,+} = \frac{1}{2} \sum_{\sigma\in\mathcal{E}} q_\sigma \left(\left(v_{\sigma,+} - v_{\sigma,-}\right)^2 + \left(v_{\sigma,+}^2 - v_{\sigma,-}^2\right) \right), \tag{42}$$

we therefore have

$$\sum_{\sigma\in\mathcal{E}} q_\sigma \left(v_{\sigma,+}^2 - v_{\sigma,-}^2\right) = \sum_{i\in\mathcal{T}} \left(\int_i \mathbf{q} \cdot \mathbf{n}_{i,\sigma} d\sigma \right) v_i^2 = \int_\Omega \nabla \cdot \mathbf{q}(\mathbf{x})\, v_{\mathcal{T}}^2\,(\mathbf{x}) dx = 0, \tag{43}$$

since we have assumed divergence-free flow. Then

$$b_h^2(v_h, v_h) \geq 0. \tag{44}$$

We also have

$$b_h^3(v_h, v_h) = c_0 \|v_h\|_{0,h} \geq 0, \tag{45}$$

therefore

$$a_h(v_h, v_h) \geq C_5 \, \|v_{_h}\|_{1,\mathcal{T}}^2 \qquad \forall v_h \in V_h. \tag{46}$$

$\square$

The following V_h- ellipticity of a_h implies that $-A_h$ is a sectorial on $L^2(\Omega)$ (uniformly in h) i.e. there exists C_1, $\theta \in (\frac{1}{2}\pi, \pi)$, such that

$$\|(\lambda I + A_h)^{-1}\|_{L(L^2(\Omega))} \leq \frac{C_1}{|\lambda|}, \qquad\qquad \lambda \in S_\theta, \tag{47}$$

where $S_\theta = \left\{\lambda \in \mathbb{C} : \lambda = \rho e^{i\phi},\ \rho > 0,\ 0 \leq |\phi| \leq \theta\right\}$.

The discrete operator $-A_h$ therefore is the infinitesimal generator of bounded analytic semigroup (or exponential operator) $S_h(t) := e^{-t\,A_h}$ on V_h such that

$$S_h(t) := e^{-t\,A_h} = \frac{1}{2\pi i}\int_{\mathcal{C}'} e^{t\,\lambda}(\lambda I + A_h)^{-1} d\lambda\ , \qquad\qquad t > 0 \tag{48}$$

where $\mathcal{C}'$ denotes a path that surrounds the spectrum of $-A_h$. As for the continuous case, Duhamel's principle implies that the solution of (27) is represented by the following integral equations (mild form)

$$X_h(t) = S_h(t)X_{0h} + \int_0^t S_h(t-s)P_hR(X_h(s))ds, \qquad\qquad t \in [0,T]\,. \tag{49}$$

For simplicity we consider a constant time-step $\Delta t > 0$. At time $t_m = m\Delta t \in [0, T]$, the mild solution (49) is given by

$$X_h(t_m) = S_h(t_m)X_{0h} + \int_0^{t_m} S_h(t_m - s)P_hR(X_h(s))ds. \tag{50}$$

Then, given the solution X_h at the time t_m, we can construct the corresponding solution at t_{m+1} as

$$X_h(t_{m+1}) = S_h(\Delta t)X_h(t_m) + \int_0^{\Delta t} S_h(\Delta t - s)P_h R(X_h(t_m + s))ds. \qquad (51)$$

Note that the expression in (51) is still an exact form of X_h. The idea behind exponential time differencing is to approximate $P_h R(X_h(t_m+s))$ by a suitable polynomial [13, 14]. We consider the simplest case where $P_h R(X_h(t_m+s))$ is approximated by the constant $P_h R(X_h(t_m))$ and the corresponding scheme (ETD1) is given by

$$X_h^{n+1} = e^{-\Delta t A_h} X_h^n + \Delta t \varphi_1(-\Delta t A_h) P_h R(X_h^m, t_m) \qquad (52)$$

where

$$\varphi_1(-\Delta t A_h) = (-\Delta t\, A_h)^{-1}\left(e^{-\Delta t A_h} - I\right) = \frac{1}{\Delta t}\int_0^{\Delta t} e^{-(\Delta t - s)A_h} ds.$$

Note that the ETD1 scheme in (52) can be rewritten as

$$X_h^{m+1} = X_h^m + \Delta t \varphi_1(-\Delta t A_h)(-A_h X_h^m + P_h R(X_h^m)). \qquad (53)$$

This new expression has the advantage that it is computationally more efficient as only one matrix exponential function needs to be evaluated at each step.

5. Main result

5.1. Convergence Theorem

We assume that the unique mild solution X of ADR problem (2) is the classical solution of (2) i.e. X is twice continuously differentiable with respect to $\mathbf{x}$ and differentiable with respect to t. This assumption is necessary to achieve optimal orders of convergence in time and space.

Theorem 5.1. *Consider the mild solution X of the ADR (2) and the numerical solution (53) given by the ETD1 scheme. Assume that Assumption 4.2 is satisfied and the reaction function R satisfies Assumption 2.1. Set $X_{0h} = P_h X_0$, assume that $X_0 \in \mathcal{D}(A)$, then the following estimate holds:*

$$\|X(t_m) - X_h^m\|_{0,h} \leq C\left(\Delta t + h\right),$$

where $C = C(\Omega, X, R, \mathbf{D}, \mathbf{q}, T, \zeta_1, \zeta_2)$.

The proof follows in Section 5.3, but we need some preparatory results first.

5.2. Preparatory results

Proposition 5.2. [***Interpolation error***]

Let $\mathcal{T}$ be an admissible mesh in the sense of Definition 3.1 and $\mathcal{T}_h$ its dual Delaunay triangulation ($\{x_i\}$ are vertices of $\mathcal{T}_h$) . Let $I_h : C(\overline{\Omega}) \rightarrow V_h$ defined by

$$I_h(u) = \sum_{i \in \mathcal{T}} u(\mathbf{x}_i)\varphi_{\mathbf{x}_i}, \qquad u \in C(\overline{\Omega}) \tag{54}$$

where $\{\varphi_{\mathbf{x}_i}\}_{i\in\mathcal{T}}$ is the nodal basis corresponding to $\{\mathbf{x}_i\}_{i\in\mathcal{T}}$ in the sense of finite element method ($\varphi_{x_i}(x_j) = \delta_{i,j}$). If $u \in C^2(\overline{\Omega})$, then there exists a positive constant $C_0(u)$ such that the following estimate holds

$$\|u - I_h(u)\| \leq C_0(u)h^2. \tag{55}$$

If $u \in C([0,T], C^2(\overline{\Omega}))$, then

$$\|u(t) - I_h(u(t))\| \leq C_0(u,T)h^2, \qquad \forall t \in [0,T]. \tag{56}$$

Proof. See [27, Section 3.4, Theorem 3.29, page 139 or Exercise 3.25 page 147] or [21, Theorem 17.1, page 132]. □

Proposition 5.3. ***[Smoothing properties of the semi group[23]]*** *Let $\beta \geq 0$ and $0 \leq \gamma \leq 1$, then there exists $C > 0$ such that*

$$\begin{aligned} \|A^\beta S(t)\|_{L(L^2(\Omega))} &\leq Ct^{-\beta} \quad \text{for} \quad t > 0, \\ \|A^{-\gamma}(I - S(t))\|_{L(L^2(\Omega))} &\leq Ct^{\gamma} \quad \text{for} \quad t \geq 0. \end{aligned}$$

In addition, the following results hold

$$A^\beta S(t) = S(t)A^\beta \quad \text{on} \quad \mathcal{D}(A^\beta).$$

$$\text{If} \quad \beta \geq \gamma \quad \text{then} \quad \mathcal{D}(A^\beta) \subset \mathcal{D}(A^\gamma).$$

$$\|D_t^l S(t)v\|_\beta \leq Ct^{-l-(\beta-\alpha)/2}\|v\|_\alpha, \;\; t > 0, \; v \in \mathcal{D}(A^{\alpha/2}) \;\; l = 0, 1,$$

where $D_t^l := \dfrac{d^l}{dt^l}$, $\|.\|_\alpha := \|A^{\alpha/2}.\|$.

Lemma 5.4. *Let X be the mild solution of (2) given in (13). Let $t_1, t_2 \in [0,T]$, $t_1 < t_2$. The following estimates hold:*

- *(i) If $X_0 \in \mathcal{D}(A)$ then*

$$\|X(t_2) - X(t_1)\| \leq C(t_2 - t_1)^{1-\epsilon} \left(\|X_0\|_2 + \sup_{0 \leq s \leq T} \|R(X(s))\| \right),$$

for $\epsilon \in (0, 1/2)$ small enough.

- *(ii) If $X_0 \in \mathcal{D}(A)$ and R satisfies the Lipschitz condition in (12) then*

$$\|X(t_2) - X(t_1)\| \leq C(t_2 - t_1) \left(\|X_0\|_2 + \sup_{0 \leq s \leq T} \|R(X(s))\| \right).$$

Proof. **Part (i)**.

Consider the difference

$$\begin{aligned} & X(t_2) - X(t_1) \\ &= (S(t_2) - S(t_1)) X_0 + \left(\int_0^{t_2} S(t_2 - s) R(X(s)) ds - \int_0^{t_1} S(t_1 - s) R(X(s)) ds \right) \\ &= I + II, \end{aligned} \tag{57}$$

so that $\|X(t_2) - X(t_1)\| \leq \|I\| + \|II\|$. We estimate each of the terms $\|I\|$ and $\|II\|$. For $\|I\|$, using Proposition 5.3 yields

$$\|I\| = \|S(t_1) A^{-1} (\mathrm{I} - S(t_2 - t_1)) A^1 X_0\| \leq C(t_2 - t_1) \|X_0\|_2.$$

For the term II, we have

$$\begin{aligned} II &= \int_0^{t_1} (S(t_2 - s) - S(t_1 - s)) R(X(s)) ds + \int_{t_1}^{t_2} S(t_2 - s) R(X(s)) ds \\ &= II_1 + II_2, \end{aligned}$$

with

$$\|II\| \leq \|II_1\| + \|II_2\|.$$

We now estimate each term $\|II_1\|$ and $\|II_2\|$. For $\|II_1\|$

$$\begin{aligned} \|II_1\| &= \| \int_0^{t_1} (S(t_2 - s) - S(t_1 - s)) R(X(s)) ds \| \\ &\leq \int_0^{t_1} \|(S(t_2 - s) - S(t_1 - s)) R(X(s))\| ds \\ &\leq \left(\int_0^{t_1} \|(S(t_2 - s) - S(t_1 - s))\|_{L(L^2(\Omega))} ds \right) \left(\sup_{0 \leq s \leq T} \|R(X(s))\| \right). \end{aligned}$$

For $\epsilon \in (0,1/2)$ small enough, using Proposition 5.3 yields

$$\begin{aligned}
\|II_1\| &\le \left(\int_0^{t_1} \|S(t_1-s)A^{1-\epsilon}A^{-1+\epsilon}(\mathrm{I}-S(t_2-t_1))\|_{L(L^2(\Omega))}ds\right)\left(\sup_{0\le s\le T}\|R(X(s))\|\right)\\
&\le \left(\int_0^{t_1} \|A^{1-\epsilon}S(t_1-s)A^{-1+\epsilon}(\mathrm{I}-S(t_2-t_1))\|_{L(L^2(\Omega))}ds\right)\left(\sup_{0\le s\le T}\|R(X(s))\|\right)\\
&\le C(t_2-t_1)^{1-\epsilon}\left(\int_0^{t_1}(t_1-s)^{-1+\epsilon}ds\right)\left(\sup_{0\le s\le T}\|R(X(s))\|\right)\\
&\le C(t_2-t_1)^{1-\epsilon}\left(\sup_{0\le s\le T}\|R(X(s))\|\right).
\end{aligned}$$

For $\|II_2\|$, using the fact that the semigroup is bounded, we have

$$\begin{aligned}
\|II\| &= \|\int_{t_1}^{t_2} S(t_2-s)R(X(s))ds\|\\
&\le \left(\int_{t_1}^{t_2}\|S(t_2-s)R(X(s))\|ds\right)\\
&\le \left(\int_{t_1}^{t_2}\|R(X(s))\|ds\right)\\
&\le C(t_2-t_1)\left(\sup_{0\le s\le T}\|R(X(s))\|\right).
\end{aligned}$$

Hence

$$\|II\| \le \|II_1\| + \|II_2\|) \le C(t_2-t_1)^{1-\epsilon}\left(\sup_{0\le s\le T}(\|R(X(s))\|)\right).$$

Combining previous estimations of $\|I\|$ and $\|II\|$ ends the proof of part (i).

Proof of part (ii) We consider again the difference in (57). The difference with the proof of part (i) comes from the estimation of II_1. This time we write

$$\begin{aligned}
II_1 &= \int_0^{t_1}(S(t_2-s)-S(t_1-s))R(X(s))ds\\
&= \int_0^{t_1}(S(t_2-s)-S(t_1-s))\left(R(X(s))-R(X(t_1))\right)ds\\
&+ \int_0^{t_1}(S(t_2-s)-S(t_1-s))R(X(t_1))ds\\
&= II_{11}+II_{12}.
\end{aligned}$$

If R satisfies the Lipschitz condition given in (12), then using the result in part (i) together with Proposition 5.3 yields

$$\begin{aligned}
\|II_{11}\| &\leq \left(\int_0^{t_1} \|S(t_2-s)-S(t_1-s)\|_{L(L^2(\Omega))}\|R(X(s))-R(X(t_1)\|ds\right)\\
&\leq C\left(\int_0^{t_1} \|S(t_2-s)-S(t_1-s)\|_{L(L^2(\Omega))}\|X(s)-X(t_1)\|ds\right)\\
&\leq C\left((t_2-t_1)\int_0^{t_1}(t_1-s)^{-\epsilon}ds\right)\\
&\leq C\,(t_2-t_1)\,,
\end{aligned}$$

for $\epsilon \in (0,1/2)$ small enough. We also have

$$\begin{aligned}
\|II_{12}\| &\leq \|R(X(t_1)\|\|\int_0^{t_1}(S(t_2-s)-S(t_1-s))ds\|_{L(L^2(\Omega))}\\
&\leq C\|\int_0^{t_1} S(t_2-s)-S(t_1-s)ds\|_{L(L^2(\Omega))}.
\end{aligned}$$

Using the two transformations $y=t_2-s,\ y=t_1-s$ we find

$$\begin{aligned}
\|II_{12}\| &= C\|\int_{t_2-t_1}^{t_2} S(y)dy-\int_0^{t_1} S(y)dy\|_{L(L^2(\Omega))}\\
&= C\|\int_{t_2-t_1}^{t_1} S(y)dy+\int_{t_1}^{t_2} S(y)dy-\int_0^{t_1} S(y)dy\|_{L(L^2(\Omega))}\\
&= C\|\int_{t_1}^{t_2} S(y)dy-\int_0^{t_2-t_1} S(y)dy\|_{L(L^2(\Omega))}\\
&\leq C(t_2-t_1).
\end{aligned}$$

The estimate of II_1 ends the proof. □

Lemma 5.5. *[Discrete Gronwall lemma [28]]*
Let the sequence $t_n = n\Delta t \leqslant T$. If the sequence of nonnegative numbers ϵ_n satisfies the inequality

$$\epsilon_n \leqslant a\,\Delta t \sum_{j=1}^{n-1} t_{n-j}^{-\beta}\epsilon_j + b\,t_n^{-\sigma}, \tag{58}$$

for $0 \leqslant \beta,\sigma < 1$ and $a, b \geqslant 0$, then the following estimate holds:

$$\epsilon_n \leqslant C\,b\,t^{-\sigma} \tag{59}$$

where the constant C depends on β,σ,a,T.

5.3. Proof of Theorem 5.1

In the followng proof, C_i and C'_i, $i = 1, \cdots, 6$ are positive constants.

Proof. We use the equivalence of the norms $\|.\|$ and $\|.\|_{0,h}$ in V_h as the mesh $\mathcal{T}$ is regular [27].

Using the triangle inequality yields

$$\begin{aligned}\|X(t_m) - X_h^m\|_{0,h} &\leq \|X(t_m) - X_h(t_m)\|_{0,h} + \|X_h(t_m) - X_h^m\|_{0,h} \\ &= I + II. \end{aligned} \tag{60}$$

Let us estimate I. Integrating the shifted version (by adding $c_0 X$ in both size) of equation (2) over each control volume $i \in \mathcal{T}$ and using the divergence theorem yields

$$\int_i X_t(\mathbf{x}, t) d\mathbf{x} - \sum_{\sigma \in \mathcal{E}_i} \int_\sigma (\mathbf{D}\nabla X - \mathbf{q}X) \cdot \mathbf{n}_\sigma d\sigma + c_0 \int_i X d\mathbf{x} = \int_i R(\mathbf{x}, t, X(\mathbf{x}, t)) d\mathbf{x}. \tag{61}$$

For $t \in [0, T]$, $i \in \mathcal{T}$ and $\sigma \in \mathcal{E}_i$ using the same notation as in [7], let us set

$$\begin{cases} R_{i,\sigma}(t) = \dfrac{1}{\text{mes}(\sigma)} \left[\dfrac{\text{mes}(\sigma)\mu_\sigma}{d(i,j)} (X_i(t) - X_j(t)) + \int_\sigma \mathbf{D}\nabla X \cdot \mathbf{n}_\sigma d\sigma \right], \\ r_{i,\sigma}(t) = \dfrac{1}{\text{mes}(\sigma)} \left[q_{i,\sigma} X_{i,+} - \int_\sigma \mathbf{q}X(t) \cdot \mathbf{n}_\sigma \right], \\ \rho_i(t) = X(\mathbf{x}_i, t) - \dfrac{1}{\text{mes}(i)} \int_i X(\mathbf{x}, t) d\mathbf{x}, \\ \varrho_i(t) = \dfrac{1}{\text{mes}(i)} \int_i R(\mathbf{x}, t, X(\mathbf{x}, t)) d\mathbf{x} - R(\mathbf{x}_i, t, X_i(t)). \end{cases} \tag{62}$$

Assuming that the unique solution X of (2) is the regular, Taylor expansion yields

$$\begin{cases} X_t(\mathbf{x}, t) = X_t(\mathbf{x}_i, t) + s_i(\mathbf{x}, t), \qquad |s_i(\mathbf{x}, t)| \leq C_1 (X, T) h \\ \int_i X_t(\mathbf{x}, t) d\mathbf{x} = \text{mes}(i) X_t(\mathbf{x}_i, t) + S_i, \quad S_i = \int_i s_i(\mathbf{x}, t) d\mathbf{x}, \quad |S_i| \leq \text{mes}(i) C_1 (X, T) h. \end{cases} \tag{63}$$

Using Assumption 4.2, mainly the fact that the coefficients of the diffusion tensor $\mathbf{D}$ and the Darcy's velocity $\mathbf{q}$ are regular, we can therefore used the

following similar results in [7] for general elliptic operators

$$\begin{cases} |R_{i,\sigma}(t)| \leq C_2\left(\mathbf{D}, X, T\right) h, \\ \\ |r_{i,\sigma}(t)| \leq C_2'\left(\mathbf{q}, X, T\right) h, \\ \\ |R_{i,\sigma}(t)| + |r_{i,\sigma}(t)| \leq C_3\left(\mathbf{q}, \mathbf{D}, X, T\right) h, \\ \\ |\rho_i(t)| \leq C_3'\left(X, T\right) h. \end{cases} \tag{64}$$

Using the fact that R is differentiable with respect to X and $\mathbf{x}$, Taylor expansion respectively yields

$$\begin{aligned} &\operatorname{mes}(i)\varrho_i(t) \\ &= \int_i R(\mathbf{x}, t, X(\mathbf{x}, t))d\mathbf{x} - \operatorname{mes}(i)R(\mathbf{x}_i, t, X_i(t)) \\ &= \int_i \left(R(\mathbf{x}, t, X(\mathbf{x}, t)) - R(\mathbf{x}_i, t, X_i(t))\right) d\mathbf{x}, \\ &= \operatorname{mes}(i)\left(R(\mathbf{x}_i, t, X(\mathbf{x}_i, t)) - R(\mathbf{x}_i, t, X_i(t))\right) + \int_i Z_1(\mathbf{x}, t)(X(\mathbf{x}, t) - X(\mathbf{x}_i, t))d\mathbf{x} \\ &\quad + \int_i Z_2(\mathbf{x}, t)(\mathbf{x} - \mathbf{x}_i)d\mathbf{x} \\ &= \operatorname{mes}(i)\left(R(\mathbf{x}_i, t, X(\mathbf{x}_i, t)) - R(\mathbf{x}_i, t, X_i(t))\right) + \kappa(\mathbf{x}_i, t, X, R), \end{aligned}$$

where

$$Z_1(\mathbf{x}, t) = \int_0^1 \frac{\partial R}{\partial X}\left(\mathbf{x}_i + \tau(\mathbf{x} - \mathbf{x}_i), t, X(\mathbf{x}_i, t) + \tau(X(\mathbf{x}, t) - X(\mathbf{x}_i, t))\right) d\tau$$

$$Z_2(\mathbf{x}, t) = \int_0^1 \frac{\partial R}{\partial \mathbf{x}}\left(\mathbf{x}_i + \tau(\mathbf{x} - \mathbf{x}_i), t, X(\mathbf{x}_i, t) + \tau(X(\mathbf{x}, t) - X(\mathbf{x}_i, t))\right) d\tau$$

$$\kappa(\mathbf{x}_i, t, X, R) = \int_i Z_1(\mathbf{x}, t)(X(\mathbf{x}, t) - X(\mathbf{x}_i, t))d\mathbf{x} + \int_i Z_2(\mathbf{x}, t)(\mathbf{x} - \mathbf{x}_i)d\mathbf{x}.$$

If the solution X is differentiable with respect $\mathbf{x}$, one more Taylor expansion yields

$$|\kappa(\mathbf{x}_i, t, X, R)| \leq \operatorname{mes}(i)C_4(R, T, X)\, h.$$

Using the Lipschitz condition (12) yields

$$\operatorname{mes}(i)\varrho_i(t) \leq \operatorname{mes}(i)\left(C_4'(\Omega, R, T, X)|X(\mathbf{x}_i, t) - X_i(t)| + C_4(R, T, X)\, h\right). \tag{65}$$

Subtracting the first equation of (21) from (61) and using previous expressions yields

$$\left\{\begin{array}{l} \mathrm{mes}(i)\dfrac{de_i(t)}{dt} + \sum\limits_{\sigma\in\mathcal{E}_i} G_{i,\sigma}(t) + W_{i,\sigma}(t) + c_0\mathrm{mes}(i)e_i(t) \\ \qquad\qquad\qquad\qquad = \int_i \left(R(\mathbf{x},t,X(\mathbf{x},t)) - R(\mathbf{x}_i,t,X_i(t))\right) d\mathbf{x} \\ \qquad\qquad\qquad\qquad + c_0\mathrm{mes}(i)\rho_i(t) - \sum\limits_{\sigma\in\mathcal{E}_i} \mathrm{mes}(\sigma)(R_{i,\sigma} + r_{i,\sigma}) - S_i(t), \quad \forall i \in \mathcal{T} \end{array}\right. \tag{66}$$

with

$$\left\{\begin{array}{l} e_i(t) = X(\mathbf{x}_i,t) - X_i(t), \qquad t \in [0,T], \\ G_{i,\sigma}(t) = -\tau_\sigma(e_j(t) - e_i(t)), \qquad \sigma = i|j, \\ G_{i,\sigma}(t) = \tau_\sigma e_i(t), \quad \sigma \in \mathcal{E}_i \cap \partial\Omega, \\ W_{i,\sigma}(t) = q_{i,\sigma}(X(\mathbf{x}_{\sigma,+},t) - X_{\sigma,+}(t)), \end{array}\right. \tag{67}$$

and

$$\left\{\begin{array}{l} \mathbf{x}_{\sigma,+} = \left\{\begin{array}{l} \mathbf{x}_i \ \text{ if } \mathbf{q}\cdot\mathbf{n}_\sigma \geq 0, \\ \mathbf{x}_j \ \text{ if } \ \mathbf{q}\cdot\mathbf{n}_\sigma < 0, \end{array}\right. \qquad \sigma = i|j, \\ \mathbf{x}_{\sigma,+} = \left\{\begin{array}{l} \mathbf{x}_i \ \text{ if } \ \mathbf{q}\cdot\mathbf{n}_\sigma \geq 0, \\ \mathbf{x}_\sigma, \quad \mathbf{x}_\sigma \in \partial\Omega \ \text{ if } \ \mathbf{q}\cdot\mathbf{n}_\sigma < 0, \end{array}\right. \qquad \sigma \in \mathcal{E}_i \cap \partial\Omega. \end{array}\right. \tag{68}$$

Multipling equation (66) by $e_i(t)$ and summing for $i \in \mathcal{T}$ yields

$$\left\{\begin{array}{l} \sum\limits_{i\in\mathcal{T}} \left[\dfrac{\mathrm{mes}(i)}{2}\dfrac{d(e_i^2(t))}{dt} + \sum\limits_{\sigma\in\mathcal{E}_i} e_i(t)(G_{i,\sigma}(t) + W_{i,\sigma}(t)) + c_0\,\mathrm{mes}(i)e_i^2(t)\right] \\ = \sum\limits_{i\in\mathcal{T}} e_i(t)\left[\int_i \left(R(\mathbf{x},t,X(\mathbf{x},t)) - R(\mathbf{x}_i,t,X_i(t))\right) d\mathbf{x}\right] \\ + \sum\limits_{i\in\mathcal{T}} \left[c_0\,\mathrm{mes}(i)\rho_i(t)e_i(t) - \sum\limits_{\sigma\in\mathcal{E}_i} \mathrm{mes}(\sigma)e_i(t)(R_{i,\sigma}(t) + r_{i,\sigma}(t)) - e_i(t)S_i(t)\right]. \end{array}\right. \tag{69}$$

Let $e_{\mathcal{T}}(t)$ a piecewise constant function defined by

$$e_{\mathcal{T}}(t) = e_i(t), \qquad \text{for} \quad \mathbf{x} \in i, \quad i \in \mathcal{T}, \quad t \in [0, T]\,. \tag{70}$$

As in the proof of Theorem 4.3, using the fact that

$$C_5 \le \mu_\sigma \le C_5', \qquad \forall \sigma \in \mathcal{E}, \tag{71}$$

where μ_σ is defined in (17) and (16) yields

$$\left\{ \begin{array}{l} C_5 \|e_{\mathcal{T}}(t)\|^2_{1,\mathcal{T}} \le \|e_{\mathcal{T}}(t)\|^2_{1,h} \le C_5' \, \|e_{\mathcal{T}}(t)\|^2_{1,\mathcal{T}} \\ \\ \|e_{\mathcal{T}}(t)\|^2_{1,\mathcal{T}} = \sum\limits_{\sigma \in \mathcal{E}} |D_\sigma e_{\mathcal{T}}(t)|^2 \dfrac{\mathrm{mes}(\sigma)}{d_\sigma} \\ \\ \|e_{\mathcal{T}}(t)\|^2_{1,h} := \sum\limits_{i \in \mathcal{T}} \sum\limits_{\sigma \in \mathcal{E}_i} e_i(t) G_{i,\sigma}(t), \end{array} \right. \tag{72}$$

where

$$\left\{ \begin{array}{ll} |D_\sigma e_{\mathcal{T}}(t)| = |e_i(t) - e_j(t)|, & \text{if} \qquad \sigma = i|j, \\ \\ |D_\sigma e_{\mathcal{T}}(t)| = |e_i(t)|, & \text{if} \qquad \sigma \in \mathcal{E}_i \cap \partial\Omega. \end{array} \right. \tag{73}$$

Setting $e_{\sigma,+}(t) = X(\mathbf{x}_{\sigma,+}, t) - X_{\sigma,+}(t)$, as in the proof of Theorem 4.3, important results from [7] yields

$$\begin{aligned} \sum_{i \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_i} e_i(t) W_{i,\sigma}(t) &= \sum_{i \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_i} q_{i,\sigma} e_i(t) (X(\mathbf{x}_{\sigma,+}, t) - X_{\sigma,+}(t)) \\ &= \sum_{i \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_i} q_{i,\sigma} e_i(t) e_{\sigma,+}(t) \ge 0. \end{aligned} \tag{74}$$

Using (74) and (65) in the expression (69) yields

$$\left\{ \begin{array}{l} \dfrac{1}{2} \sum\limits_{i \in \mathcal{T}} \mathrm{mes}(i) \dfrac{d(e_i^2(t))}{dt} + \|e_{\mathcal{T}}(t)\|^2_{1,h} + c_0 \|e_{\mathcal{T}}(t)\|^2_{0,h} \leqslant C_4' \|e_{\mathcal{T}}(t)\|^2_{0,h} + C_4 \, h \sum\limits_{i \in \mathcal{T}} \mathrm{mes}(i) |e_i(t)| \\ \\ + c_0 C_3' \, h \sum\limits_{i \in \mathcal{T}} \mathrm{mes}(i) |e_i(t)| + \sum\limits_{i \in \mathcal{T}} \sum\limits_{\sigma \in \mathcal{E}_i} \mathrm{mes}(\sigma) e_i(t) (R_{i,\sigma}(t) + r_{i,\sigma}(t)) + C_1 \, h \sum\limits_{i \in \mathcal{T}} \mathrm{mes}(i) |e_i(t)|. \end{array} \right. \tag{75}$$

The continuity of the diffusion and advection flux at each interface yields

$$R_{i,\sigma}(t) = -R_{j,\sigma}(t), \qquad r_{i,\sigma}(t) = -r_{j,\sigma}(t), \qquad \text{for } \sigma = i|j \in \mathcal{E}_{int}.$$

Set

$$R_\sigma(t) = |R_{i,\sigma}(t)|, \ \ r_\sigma(t) = |R_{i,\sigma}(t)|, \qquad i \in \mathcal{T}, \qquad \sigma \in \mathcal{E}_{int}.$$

Using the relation (64), the Cauchy-Schwarz inequality as in [7] for stationary elliptic problems and reordering the summation over the edges yields

$$\begin{aligned}
&\sum_{i\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_i} \mathrm{mes}(\sigma) e_i(t)(R_{i,\sigma}(t) + r_{i,\sigma}(t)) \\
&\leqslant \sum_{\sigma\in\mathcal{E}} D_\sigma e_{\mathcal{T}}(t)(R_\sigma(t) + r_\sigma(t)) \\
&\leqslant \left(\sum_{\sigma\in\mathcal{E}} \frac{\mathrm{mes}(\sigma)}{d_\sigma}(D_\sigma e_{\mathcal{T}}(t))^2\right)^{\frac{1}{2}} \left(\sum_{\sigma\in\mathcal{E}} \mathrm{mes}(\sigma) d_\sigma (R_\sigma + r_\sigma)^2\right)^{\frac{1}{2}}.
\end{aligned}$$

Using the fact that $\sum_{\sigma\in\mathcal{E}} \mathrm{mes}(\sigma) d_\sigma \leqslant d \ \mathrm{mes}(\Omega))$ and relation (72) yields

$$\begin{aligned}
&\sum_{i\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_i} \mathrm{mes}(\sigma) e_i(t)(R_{i,\sigma}(t) + r_{i,\sigma}(t)) \\
&\leqslant C_3 \, h \, (\mathrm{mes}(\Omega) \, d)^{\frac{1}{2}} \|e_{\mathcal{T}}(t)\|_{1,\mathcal{T}} \\
&\leqslant (C_5)^{-1} C_3 \, h \, (\mathrm{mes}(\Omega) \, d)^{\frac{1}{2}} \|e_{\mathcal{T}}(t)\|_{1,h}.
\end{aligned} \tag{76}$$

For any constant $C > 0$, Young's inequality yields

$$\left\{ \begin{array}{l}
|C \, h \sum_{i\in\mathcal{T}} \mathrm{mes}(i) e_i(t)| = |\sum_{i\in\mathcal{T}} (C \ h \ \mathrm{mes}(i)^{\frac{1}{2}})(\mathrm{mes}(i)^{\frac{1}{2}} e_i(t))| \leqslant \frac{1}{2}\|e_{\mathcal{T}}(t)\|_{0,h}^2 + \frac{1}{2}C^2 h^2 \ \mathrm{mes}(\Omega) \\[2ex]
C \, h \|e_{\mathcal{T}}(t)\|_{1,h} \leqslant \frac{1}{2} C^2 h^2 + \frac{1}{2}\|e_{\mathcal{T}}(t)\|_{1,h}^2.
\end{array} \right. \tag{77}$$

Using expression (76) and (77) in expression (75) yields

$$\left\{ \begin{array}{l}
\frac{1}{2}\left[\sum_{i\in\mathcal{T}} \mathrm{mes}(i) \frac{d(e_i^2(t))}{dt} + \|e_{\mathcal{T}}(t)\|_{1,h}^2 + c_0 \, \|e_{\mathcal{T}}(t)\|_{0,h}^2\right] \leqslant (C_4'/2 + 1)\|e_{\mathcal{T}}(t)\|_{0,h}^2 + C_6 \, h^2 \\[2ex]
C_6 = C_6(C_1, C_3, C_3', C_4, C_5).
\end{array} \right. \tag{78}$$

Bounding the left hand side of expression (78) below yields

$$\sum_{i\in\mathcal{T}} \mathrm{mes}(i) \frac{d(e_i^2(s))}{ds} \leqslant (C_4' + 2)\|e_{\mathcal{T}}(s)\|_{0,h}^2 + 2C_6 \, h^2, \qquad \forall s \in [0, T]. \tag{79}$$

Integrating both side of expression (79) through interval $[0,t]$, $0 \le t \le T$ yields

$$\|e_{\mathcal{T}}(t)\|_{0,h}^2 \le \|e_{\mathcal{T}}(0)\|_{0,h}^2 + 2\,C_6\,T\,h^2 + (C_4' + 2)\int_0^t \|e_{\mathcal{T}}(s)\|_{0,h}^2 ds, \qquad \forall t \in [0,T]. \quad (80)$$

Applying the discrete Gronwall Lemma 5.5 yields

$$\begin{aligned} \|e_{\mathcal{T}}(t)\|_{0,h}^2 &\le C\left(\|e_{\mathcal{T}}(0)\|_{0,h}^2 + h^2\right), \\ C &= C(\Omega, X, R, \mathbf{D}, \mathbf{q}, T, \zeta_1, \zeta_2). \end{aligned} \tag{81}$$

Then

$$I = \|X(t_m) - X_h(t_m)\|_{0,h} = \|e_{\mathcal{T}}(t_m)\|_{0,h} \le C\left(\|X_0 - X_{0h}\|_{0,h} + h\right). \tag{82}$$

If $X_{0h} = P_h X_0$, we have

$$\|X_0 - X_{0h}\|_{0,h} = \|X_0 - P_h X_0\|_{0,h} \le Ch, \tag{83}$$

(see [27]), we therefore have

$$I = \|X(t_m) - X_h(t_m)\|_{0,h} = \|e_{\mathcal{T}}(t_m)\|_{0,h} \le Ch. \tag{84}$$

Let us estimate II. From (50) and (52) we have

$$X_h(t_m) = S_h(t_m)X_{0h} + \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} S_h(t_m - s) P_h R(s, X_h(s)) ds, \tag{85}$$

and

$$X_h^m = S_h(t_m)X_{0h} + \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} S_h(t_m - s) P_h R(t_k, X_h^k) ds. \tag{86}$$

The smoothing properties of the semigroup S_h in Proposition 5.3 and the equivalence $\|.\| \equiv \|.\|_{0,h}$ in V_h yields

$$\begin{aligned} \|X_h(t_m) - X_h^m\|_{0,h} &\equiv \|X_h(t_m) - X_h^m\| \\ &\le C\sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} \|P_h\left(R(s, X_h(s)) - R(t_k, X_h^k)\right)\| ds, \end{aligned}$$

and

$$
\begin{aligned}
\|X_h(t_m) - X_h^m\|_{0,h} &\leq \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} (\|P_h\left(R(s, X_h(s)) - R(s, X(s))\right)\|ds \\
&\quad + \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} \|P_h\left(R(s, X(s)) - R(t_k, X_h^k)\right)\|ds \\
&= II_1 + II_2. \qquad (87)
\end{aligned}
$$

For $s \in [0, T]$, using Proposition 5.2 yields

$$
\begin{aligned}
\|X_h(s) - X(s)\| &\leq \|X_h(s) - I_h(X(s)) + I_h(X(s)) - X(s)\| \\
&\leq (\|X_h(s) - I_h(X(s))\| + \|I_h(X(s)) - X(s)\|) \\
&\leq \left(\|X_h(s) - I_h(X(s))\| + C(X, T)h^2\right). \qquad (88)
\end{aligned}
$$

Since $X_h(s) - I_h(X(s)) \in V_h$, the equivalence $\|.\| \equiv \|.\|_{0,h}$ and the uniform estimate of the term I in $[0, T]$ yields

$$
\begin{aligned}
\|X_h(s) - I_h(X(s))\| &\equiv \|X_h(s) - I_h(X(s))\|_{0,h} \\
&= \|X_h(s) - X(s)\|_{0,h} \qquad \text{(by definition of } \|.\|_{0,h}\text{)} \\
&\leq C(\Omega, X, R, \mathbf{D}, \mathbf{q}, \zeta_1, \zeta_2)h \qquad (89)
\end{aligned}
$$

Using the Lipschitz condition (12) with (89) and (88) yields

$$
II_1 \leq C(\Omega, X, R, \mathbf{D}, \mathbf{q}, T, \zeta_1, \zeta_2)h. \qquad (90)
$$

We also have

$$
\begin{aligned}
II_2 &\leq \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} \|P_h\left(R(s, X(s)) - R(t_k, X(t_k))\right)\|ds \\
&+ \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} \|P_h\left(R(t_k, X(t_k)) - R(t_k, X_h^k)\right)\|ds \\
&= II_2^1 + II_2^2. \qquad (91)
\end{aligned}
$$

Using Lemma 5.4 and the Lipschitz condition (12) yields

$$
\begin{aligned}
II_2^1 &\leq C\sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} \|X(s) - X(t_k)\|ds \\
&\leq C\sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} (s - t_k)ds \\
&\leq C(T)\Delta t. \qquad (92)
\end{aligned}
$$

Using Lipschitz condition (12), Proposition 5.2 and the equivalence $\|.\| \equiv \|.\|_{0,h}$ in V_h

$$\begin{aligned}
II_2^2 &\leq C\sum_{k=0}^{m-1}\int_{t_k}^{t_{k+1}} \|X(t_k) - I_h(X(t_k)) + I_h(X(t_k)) - X_h^k\| ds && (93)\\
&\leq C\sum_{k=0}^{m-1}\int_{t_k}^{t_{k+1}} \|X(t_k) - I_h(X(t_k))\| + \|I_h(X(t_k)) - X_h^k\|_{0,h} ds && (94)\\
&\leq C(X,T)\left(h^2 + \sum_{k=0}^{m-1}\int_{t_k}^{t_{k+1}} \|X(t_k) - X_h^k\|_{0,h} ds\right) && (95)
\end{aligned}$$

Then

$$II \leq C\left((\Delta t + h) + \sum_{k=0}^{m-1}\int_{t_k}^{t_{k+1}} \|X(t_k) - X_h^k\|_{0,h} ds\right),$$

Combining estimates I and II yields

$$\begin{aligned}
&\|X(t_m) - X_h^m)\|_{0,h}\\
&\leq C\left(\Delta t + h + \sum_{k=0}^{m-1}\int_{t_k}^{t_{k+1}} \|X(t_k) - X_h^k\|_{0,h} ds\right). && (96)
\end{aligned}$$

Applying the discrete Gronwall Lemma 5.5 in (96) ends the proof.

□

6. Simulations

The Key point in (ETD1) scheme is the computing of the exponential function, the so called φ_1. It is well known that a standard Padé approximation for a matrix exponential is not an efficient method for large scale problems [29]. Here we use the real fast Leja points and the Krylov subspace techniques to evaluate the action of the exponential matrix function $\varphi_1(-\Delta t\, A_h)$ on a vector $\mathbf{v}$, instead of computing the full exponential function $\varphi_1(-\Delta t\, A_h)$ as in a standard Padé approximation. The details of the Krylov subspace technique are given in [18, 8, 2, 19] while more information about the real fast Leja points can be found in [20, 16, 17, 2, 19].

6.1. Space convergence

The aims here is to analyse the convergence in space by comparing the numerical solution to the exact solution for a linear problem. We consider here a linear reaction diffusion with exact solution given in [15]. The domain is defined as $\Omega = [L_0, L_1) \times [L_0, L_1)$, $L_0 = 0.01$, $L_1 = 2$. The initial time is given as $t_0 = 0.01$. This is necessary because the exact solution is not defined at the origin and at $t = 0$. The dispersion tensor $\mathbf{D}$ is diagonal and heterogeneous with coefficients given by

$$\begin{cases} D_{1,1}(x,y) = D_0 u_0^2 x^2 \quad (x,y) \quad \in \overline{\Omega} \\ D_{2,2}(x,y) = D_0 u_0^2 y^2 \quad (x,y) \quad \in \overline{\Omega}. \end{cases}$$

A curved the velocity field (Figure 2(a)) is given explicitly by

$$\begin{cases} \mathbf{q} = (q_x, q_y)^T \\ q_x(x,y) = u_0 x \quad (x,y) \quad \in \overline{\Omega} \\ q_y(x,y) = -u_0 y \quad (x,y) \quad \in \overline{\Omega} \end{cases} \tag{97}$$

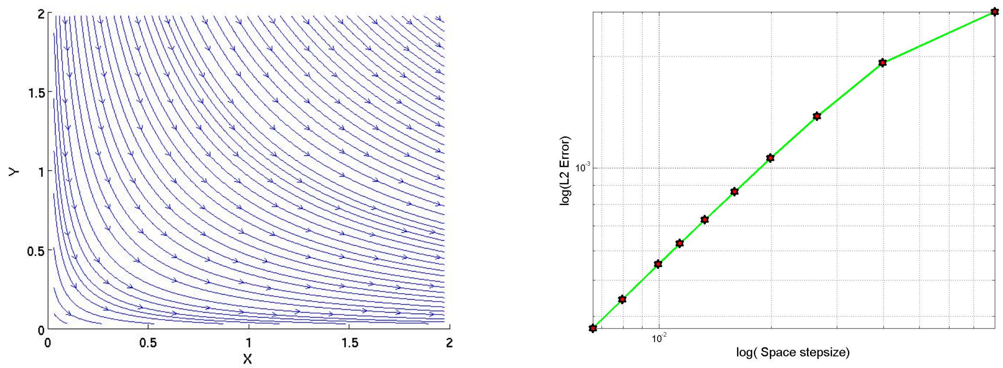
where $D_0 = 0.1$ and $u_0 = 2$. The finite volume mesh $\mathcal{T}$ is the rectangular grid. Initial and boundary conditions are taken according to the exact solution [15], assuming an instantaneous release at a point (x_0, y_0), $x_0 = 1.5$, $y_0 = 1.5$. We take a fixed time-step of $\Delta t = 1/3000$. We use here the real the fast Léja to compute the action of the exponential function φ_1. The final time here is $T = 1$.

Figure 1(b) shows a convergence of order $\mathcal{O}(h)$ for the spatial discretisation, which agrees with the predicted order in Theorem 5.1.

6.2. Time Convergence

We use the upper 40 layers of the highly heterogeneous SPE10 case, which represents a braided fluvial North Sea oil field [1] for porosity and permeability fields.

The domain is $\Omega = [0, L_1] \times [0, L_2] \times [0, L_3]$, the finite volume mesh $\mathcal{T}$ is the set of parallelepipeds with space discretization stepsize $\Delta x = 20$ ft, $\Delta y = 10$ ft and $\Delta z = 2\,\text{ft}$. Dimensions are $L_1 = 1200 ft$, $L_2 = 2200$ ft, $L_3 = 40$ ft. We use for the absolute tolerance error tol $= 10^{-6}$ and $m = 8$ for the Krylov subspace dimension.



(a) (b)

Figure 1: (a) shows the streamlines of the velocity field, (b) shows the L^2 norm of the error at $T = 1$ as a function of the grid size h for linear advection diffusion.

To have the velocity field we solve with our finite volume scheme the system

$$\begin{cases} \nabla \cdot \mathbf{q} = 0, \\ \mathbf{q} = -\dfrac{K(\mathbf{x})}{\mu} \nabla p, \end{cases} \tag{98}$$

where the dynamical viscosity is $\mu = 0.3$cp and the diagonal permeability tensor K comes from [1]. We use the Dirichlet boundary at

$$\Gamma_D = \{\{0\} \times \{0\} \times [0, L_3]\} \cup \{\{L_1\} \times \{L_2\} \times [0, L_3]\},$$

and homogenous Neumann boundary elsewhere such that

$$\begin{aligned} p &= \begin{cases} 3998.96 \ \text{psi} \quad \text{in} \quad \{0\} \times \{0\} \times [0, L_3] \\ \\ 7997.92 \ \text{psi} \quad \text{in} \quad \{L_1\} \times \{L_2\} \times [0, L_3] \end{cases} \\ -K \, \nabla p(\mathbf{x}, t) \cdot \mathbf{n} &= 0 \quad \text{in} \quad \Gamma_N = \partial\Omega \backslash \Gamma_D. \end{aligned}$$

For the nonlinear advection diffusion reaction we use the following boundary

conditions

$$
\begin{aligned}
X &= 0 \quad \text{in} \quad \{\{0\} \times \{0\} \times [0, L_3]\} \times [0, T] \\
X &= 1 \quad \text{in} \quad \{\{L_1\} \times \{L_2\} \times [0, L_3]\} \times [0, T]
\end{aligned}
$$

$$
\begin{aligned}
-(\mathbf{D}\nabla X)(\mathbf{x}, t) \cdot \mathbf{n} &= 0 \quad \text{in} \quad \Gamma_N \times [0, T] \\
X_0 &= 0 \quad \text{in} \quad \Omega \quad \text{(initial solution)}
\end{aligned}
$$

where $\mathbf{n}$ is the unit outward normal vector to Γ_N. The velocity field obtained in (98) is piecewise constant in the mesh $\mathcal{T}$. For reaction function, we use the classical Langmuir sorption isotherm given by $R(X) = \dfrac{\lambda \beta X}{1 + \lambda X}$, with $\lambda = 1$, $\beta = 10^{-3}$. This reaction function is obviously Lipschitz. The reference or 'exact' solution is the numerical solution with the smaller time step size ($\Delta t = 0.25$). The final time here is $T = 4096$ seconds. We take a uniform dispersion(diffusion) tensor of $\mathbf{D} = 10^{-6} \times \mathbf{I}_3$. Figure 2(b) shows a convergence of order $\mathcal{O}(\Delta t)$ for the time discretisation, which agrees with the predicted order in Theorem 5.1 even we don't have any information about the regularity of the exact solution. In fact to obtain the optimal order of convergence in time, the exact solution should be differentiable respect to the time, which may be the case here since the initial solution is infinitely differentiable and we are dealing with parabolic problem.

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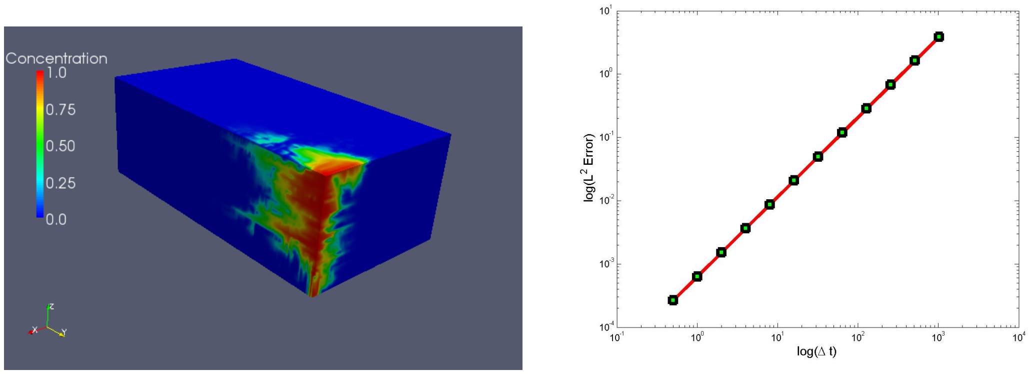

(a) (b)

Figure 2: (a) Concentration after $T = 4096$ seconds, the initial solution is $X_0 = 0$, (a) for the first upper 40 layers of the SPE 10 model, (b) shows the convergence in time, the slope which is the temporal order of convergence is $1,004$.

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